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Birch, Heidi; Andersen, Henrik Rasmus; Comber, Mike; Mayer, Philipp

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Biodegradation testing of chemicals with high Henry's constants – separating mass and effective concentration reveals higher rate constants

Heidi Birch, Henrik R. Andersen, Mike Comber, Philipp Mayer

Technical University of Denmark, Department of Environmental Engineering, Bygningstorvet, Building 115, 2800 Kgs. Lyngby, Denmark. hbir@env.dtu.dk, hran@env.dtu.dk, philm@env.dtu.dk

Mike Comber Consulting, Bridford, Exeter, UK. mike.comber42@btinternet.com

During simulation-type biodegradation tests, volatile chemicals will continuously partition between water phase and headspace. This study addressed how (1) this partitioning affects biodegradation test results and (2) it can be accounted for by combining mass balance and dynamic biodegradation models. An aqueous mixture of 9 (semi)volatile chemicals was first prepared using passive dosing and then diluted with environmental surface water to produce test systems containing concentrations in the ng/L to µg/L range. After incubation for 2 hours to 4 weeks, automated Headspace Solid Phase Microextraction (HS-SPME) was applied directly on the test systems to measure substrate depletion by biodegradation relative to abiotic controls. HS-SPME was also applied to determine air to water partitioning ratios. Water phase biodegradation rate constants, k_{water} , were up to 72 times higher than test system biodegradation rate constants, k_{system} . True water phase degradation rate constants facilitate extrapolation to other air-water systems and are more suitable input parameters for aquatic exposure and fate models. As such, they should be considered more appropriate for risk assessments than test system rate constants.

Keywords: Biodegradation, Surface water, partitioning, degradation